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ELECTRON CAPTURE BY PROTONS IN HYDROGEN IN AN ELECTRIC FIELD

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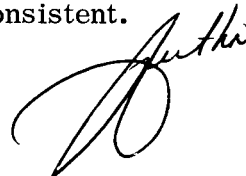# ELECTRON CAPTURE BY PROTONS IN HYDROGEN
IN AN ELECTRIC FIELD

SUMMARY

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The evaluation of the capture cross section in the Brinkman Kramers approximation with the hydrogen atom wave function in parabolic coordinates is much simpler than this wave function in spherical coordinates. A simple closed formula for the electron capture cross section in parabolic coordinates, appropriate to the charge transfer in an electric field, is derived with the electron initially and finally in two arbitrary sublevels of the atom, and it is shown that the cross section, apart from a weighting factor, is independent of the particular sublevel and depends only on the principal quantum numbers involved. In this way the charge transfer cross section in an electric field is obtained. In addition, the solution of the problem in parabolic coordinates leads, through a transformation, to the determination in closed form of the cross section is spherical coordinates. A general formula is worked out for the cross section $\sigma(nl, n'l')$, and as an example simple formulas for $\sigma(1s, ln)$ with the final states the sublevels of $n = 1, 2, 3$ are tabulated. Previous works have listed these cross sections in integral forms.

It is found that the momentum distribution of electrons in the Stark levels of the hydrogen have extremely simple form in contrast to the momentum distribution in the optical levels. The averaged momentum distribution over the sublevels of a principal quantum number gives results identical to the results originally obtained by Fock, and recently reobtained by a different method by May.

The classical momentum distribution of a bound particle in a Coulomb field is shown to be the same in form as the quantum mechanical distribution. The use of this distribution function in classical calculation of scattering will make the classical and the quantum mechanical calculations more consistent.

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I. INTRODUCTION

The momentum density distribution function for a bound electron in the Coulomb field of a nucleus of charge Ze occupying the state of the principal quantum number n and the azimuthal quantum number l has been found by Podolanski and Pauling[1] using the Fourier transform of the spatial wave functions, and by Fock[2] by solving the Schroedinger integral equation in the momentum space. Fock further has shown that when the above density distribution function is averaged over l, a simple function results. Let $\mathbf{p}$ represent the momentum of the electron and $\mathbf{q}$ its propagation vector, then $\mathbf{p} = \hbar\mathbf{q}$ and this function is given by[3]

$$D(n, \mathbf{q}) = \frac{1}{n^2} \sum_{l=0}^{n-1} (2l + 1) D(nl, \mathbf{q}) = \frac{8 Z^2 \alpha^3}{n^2 \pi^2 a_0^2} \cdot \frac{1}{(\alpha^2 + q^2)^4} ,$$

$$\alpha = \frac{Z}{n a_0}, \tag{1}$$

with a_0 the Bohr radius. Eq. (1) has recently been rederived by May[4] by a different method.

The momentum density distribution function of a bound electron in a Coulomb field has a particular simple form when the wave function is expressed in parabolic coordinates, which is the wave function of the hydrogen atom in an electric field, weak compared to the electron-nucleus interaction. If we specify a particular state of the electron by $n n_1 n_2$, with n_1 and n_2 the quantum numbers corresponding to the ξ and η coordinates, it is shown here that the momentum distribution function, except for a weighting factor, has the same form as $D(n, \mathbf{q})$ given by Eq. (1), while the same function describing a state nl in spherical coordinates has a more complicated form. It is given in terms of the Gegenbauer polynomials whose argument is a function of the q[5].

The electron capture cross section by proton from the hydrogen atom in the Born approximation in which the interaction between the nuclei is neglected is given as an integral over the product of the squared moduli of the Fourier transforms of the initial and the final electron states wave functions.[6,7] This integral is the same as an integral over the product of the momentum densities of the two states. This is the approximation used in this paper and by using momentum density functions of the Stark levels of the hydrogen atom which are similar to the density function given in Eq. (1), the integral is found in closed form. Furthermore it is found the interesting result that the capture cross section for the initial state $n\, n_1 n_2$ and the final state $n' n'_1 n'_2$ is independent of n_1, n_2, n'_1 and n'_2, and depends only on the principal quantum numbers n and n'. The other vairable parameters of the cross sections are the charges of the target nucleus and the incident particle, Z and Z', and the initial relative velocity of the two heavy particles.

In problems in which radiative transitions affect the population densities of the excited states of the hydrogen atom, and also in the capture problems in the non-hydrogenic atoms with wave functions which can be approximated by the products of the one electron wave functions, it is desirable to have the capture cross sections in spherical coordinates. Bates and Dalgarno [8] have found these cross sections between the ground state as the initial state and the sublevels of the $n = 1 - 4$ as the final states. Hiskes [9] has extended these calculations to sublevels through $n = 15$ as the final states. In all these calculations, however, the results are in integral form. By transforming the hydrogenic atom wave functions from the parabolic to the spherical coordinates wave functions, and using the electron capture amplitudes in parabooic coordinates, it is possible to express the cross section in spherical coordinates in closed form, and as a sum over finite number of terms. This has been done here and a general expression for the cross section for the initial state $n\,l$ and the final state $n'\,l'$ is derived. In particular the cross section between the ground state and all sublevels through $n = 3$ are listed.

At the end, the classical momentum distribution of a bound particle in a Coulomb field is worked out in Appendix I, and it is shown that the distribution function is similar to the quantum mechanical distribution function given by (1). By applying the Bohr-Sommerfeld quantization rule to the classical function, the two functions become identical. The consistency of the classical and the quantum mechanical distribution functions makes it desirable that in a classical calculation of some scattering problems the velocity distribution function given in Appendix I be used, and comparison be made with the available quantum mechanical calculations.

II. MOMENTUM DISTRIBUTION IN THE STARK LEVELS OF THE HYDROGEN ATOM

The Schroedinger equation for a bound electron with position vector $\mathbf{r}$ in the field of a charge Ze located at the origin is given by

$$\left[-\frac{1}{2}\nabla^2 - \frac{Z}{a_0 r}\right]\psi(\alpha, \mathbf{r}) = -\frac{1}{2}\alpha^2 \psi(\alpha, \mathbf{r}), \qquad (2)$$

with α defined in (1). The Fourier transform of $\psi(\alpha, \mathbf{r})$ is given by

$$u(\alpha, \mathbf{q}) = (2\pi)^{-3/2}\int e^{i\mathbf{q}\cdot\mathbf{r}}\psi(\alpha,\mathbf{r})d\mathbf{r}. \qquad (3)$$

We define in addition the function

$$v(\alpha, \mathbf{q}) = (2\pi)^{-3/2}\int e^{i\mathbf{q}\cdot\mathbf{r}}\frac{Z}{r}\psi(\alpha, \mathbf{r})\,d\mathbf{r}. \qquad (4)$$

Then by substituting $(Z/r)\psi(\alpha, \mathbf{r})$ from Eq. (2) into Eq. (4) and carrying out a partial integration we obtain

$$u(\alpha, \mathbf{q}) = \frac{2}{a_0(\alpha^2 + q^2)}\,v(\alpha, \mathbf{q}). \qquad (5)$$

The momentum density, and also the electron capture cross sections, are given in terms of the squared modulus of $u(\alpha, \mathbf{q})$ summed over the magnetic quantum numbers. Since this quantity is a scalar and invariant under rotation

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of the coordinate system, for evaluation of $u(\alpha, \mathbf{q})$ we can take for convenience the z-axis of the coordinate system along the $\mathbf{q}$ and we designate in this case the $u(\alpha, \mathbf{q})$ and $v(\alpha, \mathbf{q})$ by $u(\alpha, q)$ and $v(\alpha, q)$ respectively.

We now evaluate $v(\alpha, q)$ in the parabolic coordinates. Keeping in mind that in these coordinates $r = 1/2(\xi + \eta)$, $z = 1/2(\xi - \eta)$, $d\mathbf{r} = 1/4 (\xi + \eta) d\xi d\eta d\phi$, and expressing the spacial wave function as the product of two associated Laguerre functions[10], we obtain from (4):

$$v(nn_1 n_2 m, q) = (2\pi)^{-3/2} \int e^{iqz} \frac{Z}{r} \psi(nn_1 n_2 m, \mathbf{r}) d\mathbf{r} = 0, \; m \neq 0 , \qquad (6)$$

$$v(nn_1 n_2 o, q) = (2\pi)^{-3/2} \int e^{iqz} \frac{Z}{r} \psi(nn_1 n_2 o, \mathbf{r}) d\mathbf{r}$$

$$= \frac{1}{2\pi \sqrt{2n}} \cdot \frac{Z\alpha^{3/2}}{n_1! n_2!} \int_0^\infty \int_0^\infty \exp\left[-\frac{\alpha}{2}(\xi + \eta) + \frac{iq}{2}(\xi - \eta)\right] L_{n_1}^0 (\alpha\xi) L_{n_2}^0 (\alpha\eta) d\xi d\eta$$

$$= \frac{1}{2\pi\sqrt{2n}} \cdot \frac{Z\alpha^{3/2}}{n_1! n_2!} I(n_1) I^*(n_2), \qquad (7)$$

where

$$I(l) = \int_0^\infty \exp\left[-\left(\frac{\alpha}{2} - \frac{iq}{2}\right) \xi\right] L_l^0 (\alpha\xi) d\xi. \qquad (8)$$

Using the generating function of the associated Laguerre functions[11] it follows from (8) that

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$$\sum_{l=0}^{\infty} \frac{s^l \, I(l)}{l \, !} = \frac{1}{1-s} \int_0^{\infty} \exp\left[-\left(\frac{\alpha}{2} - \frac{iq}{2} + \frac{\alpha s}{1-s}\right) \xi\right] dx$$

$$= \left[\frac{1}{2}(\alpha - iq)(1-s) + \alpha s\right]^{-1}. \tag{9}$$

Now by introducing

$$\omega = \frac{1}{2}(\alpha - iq), \tag{10}$$

the preceding equation can be written

$$\sum_{l=0}^{\infty} \frac{s^l \, I(l)}{l \, !} = \frac{1}{\omega + \omega^* s} = \omega^{-1} \sum_{l=0}^{\infty} \left(\frac{-\omega^*}{\omega}\right)^l s^l \tag{11}$$

By equating the coefficients of equal powers of s on both sides of this equation we obtain

$$I(l) = \frac{l \, !}{\omega} \left(-\frac{\omega^*}{\omega}\right)^l. \tag{12}$$

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Substitution of $I(l)$ from this equation into Eq. (7) gives

$$v(nn_1n_2o, q) = \frac{1}{2\pi\sqrt{2n}} \frac{Z\alpha^{3/2}}{|\omega|^2} \left(-\frac{\omega*}{\omega}\right)^{n_1-n_2}. \tag{13}$$

By making use of the equation

$$n_1 + n_2 = n - 1 - m, \tag{14}$$

Eq. (13) can be written, after neglecting a constant phase factor,

$$v(nn_1n_2o, q) = \frac{1}{2\pi\sqrt{2n}} \frac{Z\alpha^{3/2}}{|\omega|^2} \left(\frac{\omega*}{\omega}\right)^{2n_1}, \tag{15}$$

and by Eqs. (5, 10),

$$u(nn_1n_2o, q) = \frac{1}{2\pi\sqrt{2n}} \frac{Z\alpha^{3/2}}{2a_0|\omega|^4} \left(\frac{\omega*}{\omega}\right)^{2n_1}. \tag{16}$$

Equations (15, 16) are the main equations from which the momentum distribution and electron capture cross sections are derived.

The momentum distribution of an electron in the state nn_1n_2 is given by

$$D(nn_1n_2, \mathbf{q}) = \sum_m |u(nn_1n_2m, \mathbf{q})|^2$$

$$= |u(nn_1n_20, q)|^2 = \frac{8 Z^2 \alpha^3}{n \pi^2 a_0^2} \cdot \frac{1}{(\alpha^2 + q^2)^4}, \qquad (17)$$

an expression which is independent of the sublevel quantum numbers n_1 and n_2.

The averaged momentum distribution of an electron in the shell n is given by averaging $D(nn_1 n_2, \mathbf{q})$ over all n_1 and n_2. Keeping in mind that there are n^2 states for a given n we obtain

$$D(n, \mathbf{q}) = n^{-2} \sum_{n_1=0}^{n-1} D(nn_1n_2, \mathbf{q}) = n^{-1} D(nn_1n_2, \mathbf{q})$$

$$= \frac{8 Z^2 \alpha^3}{n^2 \pi^2 a_0^2} \cdot \frac{1}{(\alpha^2 + q^2)^4}. \qquad (18)$$

It is interesting to notice that the integral with respect to $\mathbf{q}$ over $D(n, \mathbf{q})$ is normalized to unity which corresponds to an electron in the n shell:

$$\int D(n, \mathbf{q}) \, d\mathbf{q} = \frac{32 Z^2 \alpha^3}{n^2 \pi a_0^2} \int_0^\infty \frac{q^2 \, dq}{(\alpha^2 + q^2)^4}$$

$$= \frac{32 Z^2 \alpha^3}{n^2 \pi a_0^2} \cdot \frac{\pi}{32 \alpha^5} = 1. \qquad (19)$$

The expression for $D(n, \mathbf{q})$ given in Eq. (18) is identical to the expression given in Eq. (1), derived by Fock and May using spherical coordinates, and to the expression given in Eq. (A11) for the classical momentum distribution in a Coulomb field.

Equation (17) has the interesting meaning that the Stark levels of the hydrogen atom within a given shell n, except for a weighting factor, have the same momentum distribution.

III. CAPTURE CROSS SECTION IN AN ELECTRIC FIELD [12]

Assume a nucleus of charge Z' and mass M' captures an electron from a single electron atom with nucleus of charge Z and mass M to form an atom with nucleus of charge Z' and mass M'. The capture cross section in the Born approximation in which the interaction between the nuclei is neglected is given by[8,13]

$$\sigma(i, f) = \frac{2\pi \mu^2 e^2}{\hbar^4} \frac{v'}{v} \int_{-1}^{+1} |f(\alpha, \mathbf{q})|^2 \times |g(\alpha', \mathbf{q}')|^2 \, d(\cos \theta), \quad (20)$$

with μ the reduced mass of the system, e the absolute value of the electronic charge, v and v' the magnitudes of the initial and final velocities of relative motion of the nuclei; and θ the angle between $\mathbf{v}$ and $\mathbf{v}'$. From here on the unprimed symbols correspond to the initial states while the primed are for the final states. The functions $f(\alpha, \mathbf{q})$ and $g(\alpha, \mathbf{q})$ are defined by

$$f(\alpha, \mathbf{q}) = \int e^{i\mathbf{q} \cdot \mathbf{r}} \psi(\alpha, \mathbf{r}) \, d\mathbf{r}, \quad (21)$$

$$g(\alpha, \mathbf{q}) = \int e^{i\mathbf{q} \cdot \mathbf{r}} \frac{Z}{r} \psi(\alpha, \mathbf{r}) \, d\mathbf{r}, \quad (22)$$

with $\psi(\alpha, \mathbf{r})$ and $\psi(\alpha', \mathbf{r}')$ the wave functions of the atoms Z and Z', and $\mathbf{q}$ and $\mathbf{q}'$ are related to the velocities $\mathbf{v}$ and $\mathbf{v}'$ through

$$\mathbf{q} = \frac{M}{M + m} \mathbf{k} - \mathbf{k}', \quad \mathbf{q}' = \mathbf{k} - \frac{M'}{M' + m} \mathbf{k}', \quad (23)$$

with

$$\mathbf{k} = \frac{M'(M + m)}{\hbar(M' + M + m)} \mathbf{v}, \quad \mathbf{k}' = \frac{M(M' + m)}{\hbar(M' + M + m)} \mathbf{v}'. \quad (24)$$

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In the impact parameter approximation the corresponding expression for the cross section is given by[4,14,15]

$$\sigma(i, f) = \frac{1}{2\pi p^2} \int_0^\infty |f(\alpha, q)|^2 \times |g(\alpha', q')|^2 \, \rho d\rho, \qquad (25)$$

with p a dimensionless quantity defined by

$$p = \hbar v/e^2, \qquad (26)$$

and

$$q^2 = \rho^2 + q_z^2, \quad q'^2 = \rho^2 + q_z'^2 \qquad (27)$$

with

$$q_z \equiv \beta = \frac{1}{2a_0 p}\left[p^2 - \left(\frac{Z^2}{n^2} - \frac{Z'^2}{n'^2}\right)\right], \quad q_z' \equiv \beta' = \frac{-1}{2a_0 p}\left[p^2 + \left(\frac{Z^2}{n^2} - \frac{Z'^2}{n'^2}\right)\right], \qquad (28)$$

with a_0 the Bohr radius and n and n' the principal quantum numbers of the initial and the final states of the electron.

As the integral that appears in the impact parameter method is easier to handle, the cross sections evaluated below are according to this method.

In a weak electric field the energy levels of the hydrogen atom split into Stark levels. The corresponding wave functions are given in parabolic coordinates. By the definitions (21, 22) and through Eqs. (15, 16) we obtain

$$f(nn_1n_2 o, q) = \sqrt{\frac{\pi}{n}} \frac{Z\alpha^{3/2}}{2a_0 |\omega|^4}\left(\frac{\omega^*}{\omega}\right)^{2n_1}, \qquad (29)$$

$$g(nn_1n_2 o, q) = \sqrt{\frac{\pi}{n}} \frac{Z\alpha^{3/2}}{|\omega|^2}\left(\frac{\omega*}{\omega}\right)^{2n_1}, \qquad (30)$$

The capture cross section in the impact parameter approximation with the atom Z in the state nn_1n_2 and the atom Z' in the state $n'n_1'n_2'$ is then given by

$$\sigma(nn_1n_2, n'n_1'n_2') = \frac{2\pi Z^2 Z'^2 (aa')^3}{16nn' a_0^2 p^2} \int_0^\infty \frac{\rho d\rho}{|\omega|^8 \times |\omega'|^4} \tag{31}$$

Since through Eqs. (10, 1, 27, 28) we have

$$|\omega'|^2 = \frac{1}{4}(a'^2 + q'^2) = \frac{1}{4}(a^2 + q^2) = |\omega|^2, \tag{32}$$

it follows that

$$\sigma(nn_1n_2, n'n_1'n_2') = \frac{2^9 \pi (ZZ')^2 (aa')^3}{nn' a_0^2 p^2} \int_0^\infty \frac{\rho d\rho}{[a^2 + \beta^2 + \rho^2]^6}$$

$$= \pi a_0^2 \frac{2^8 (ZZ')^5}{5(nn')^4 p^2} \cdot \frac{1}{[(a^2 + \beta^2) a_0^2]^5}. \tag{33}$$

It is evident that as stated previously $\sigma(nn_1n_2, n'n_1'n_2')$ is independent of $n_1 n_2 n_1' n_2'$. The transition $\sigma(nn_1n_2, n')$ is obtained by summing $\sigma(nn_1n_2, n'n_1'n_2')$ over $n_1'n_2'$. Noticing that only states with $m' = 0$ contribute to the cross section we obtain

$$\sigma(nn_1n_2, n') = n' \sigma(nn_1n_2, n'n_1'n_2')$$

$$= \pi a_0^2 \frac{2^8 (ZZ')^5}{5n^4 n'^3 p^2} \cdot \frac{1}{[(a^2 + q_z^2) a_0^2]^5}. \tag{34}$$

Finally the transition $\sigma(n, n')$ is obtained by averaging $\sigma(nn_1n_2, n')$ over the initial states. Since there are n^2 initial states but only n states have nonvanishing cross sections we obtain

$$\sigma(n, n') = n^{-1} \sigma(nn_1n_2, n')$$

$$= \pi a_0^2 \frac{2^8 (ZZ')^5}{5n^5 n'^3 p^2} \cdot \frac{1}{[(a^2 + q_z^2) a_0^2]^5}. \tag{35}$$

The above result is identical with the result obtained by May.[4]

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IV. Capture Cross Section in Spherical Coordinates

Let $\varphi(n\,l\,m\,|\,\mathbf{r})$ represent the wave function of the hydrogen atom in spherical coordinates. Then we define the functions $F(n\,l\,m,\,\mathbf{q})$ and $G(n\,l\,m,\,\mathbf{q})$ by

$$F(n\,l\,m,\,\mathbf{q}) = \int e^{i\mathbf{q}\cdot\mathbf{r}}\,\varphi(n\,l\,m,\,\mathbf{r})\,d\mathbf{r}, \tag{36}$$

$$G(n\,l\,m,\,\mathbf{q}) = \int e^{i\mathbf{q}\cdot\mathbf{r}}\,\frac{Z}{r}\,\varphi(n\,l\,m,\,\mathbf{r})\,d\mathbf{r}. \tag{37}$$

By writing

$$\varphi(n\,l\,m,\,\mathbf{r}) = R_{nl}(r)\,Y_{l\,m}(\hat{\mathbf{r}}), \tag{38}$$

and using the expansion[16]

$$\exp[i\,\mathbf{q}\cdot\mathbf{r}] = 4\pi \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} i^{\lambda}\,j_{\lambda}(qr)\,Y_{\lambda\mu}(\hat{\mathbf{q}})\,Y_{\lambda\mu}^{*}(\hat{\mathbf{r}}) \tag{39}$$

where $\hat{\mathbf{r}}$ and $\hat{\mathbf{q}}$ are unit vectors in the directions of $\mathbf{q}$ and $\mathbf{r}$, Eq. (36) can be written as

$$F(n\,l\,m,\mathbf{q}) = 4\pi\,i^{l}\,I_{nl}(q)\,Y_{l\,m}(\hat{\mathbf{q}}), \tag{40}$$

where

$$I_{nl}(q) = \int_{0}^{\infty} R_{nl}(r)\,j_{l}(qr)\,r^2\,dr \tag{41}$$

When $\hat{\mathbf{q}}$ is along the z axis, by the definition of $Y_{l\,m}(\hat{\mathbf{q}})$ in terms of the associated Legendre polynomials we have

$$Y_{l\,m}(\hat{\mathbf{q}} = \hat{\mathbf{z}}) = \sqrt{\frac{2l+1}{4\pi}}\,\delta(m,\,0). \tag{42}$$

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If in this case as usual we designate the $F(n\,l\,m, \mathbf{q})$ by $F(n\,l\,m, q)$, through Eq. (40) we obtain

$$F(n\,l\,m, q) = \delta(m, o)\, 4\pi\, i^l \sqrt{\frac{2l+1}{4\pi}}\, I_{nl}(q), \qquad (43)$$

and

$$F(n\,l\,m, \mathbf{q}) = \sqrt{\frac{4\pi}{2l+1}}\, F(n\,l\,o, q)\, Y_{lm}(\hat{\mathbf{q}}). \qquad (44)$$

When Eq. (44) is summed over m and use is made of[17]

$$\sum_{m=-l}^{l} |Y_{lm}(\hat{\mathbf{q}})|^2 = \frac{2l+1}{4\pi}, \qquad (45)$$

we obtain

$$\sum_{m=-l}^{l} |F(n\,l\,m, \mathbf{q})|^2 = F(n\,l\,o, q). \qquad (46)$$

This was the result stated at the beginning of Sec. II by the statement that the left hand side of Eq. (46) is a scalar and invariant under rotation of the coordinate system.

Since the wave function of the hydrogen atom forms a complete set in each of the two spherical and parabolic coordinates, the wave function in spherical coordinates can be expressed as a linear superposition of the wave functions in parabolic coordinates. In this transformation the principal and the magnetic quantum numbers n and m remain fixed:

$$\varphi(n\,l\,m, \mathbf{r}) = \sum_{n_1=0}^{n-1-m} a_{l\,n_1}\, \psi(n n_1 n_2 m, \mathbf{r}), \qquad (47)$$

where $a_{l\,n_1}$ are the elements of the transformation matrix. In our problem m = 0. By dropping nm from the indices in Eq. (47), replacing n_1 by i, substituting this equation in Eq. (36) and making use of Eq. (21) we obtain

$$F(l, q) = \sum_{i=0}^{n-1} a_{l\,i}\, f(i, q). \qquad (48)$$

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The determination of $a_{l\,i}$ for $m = 0$ and arbitrary n is worked out in Appendix II, and the matrices for $n = 1, 2, 3, 4, 5$ are given explicitly.

By Eq. (29) we now obtain

$$|F(l,\, q)|^2 = \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} a_{l\,i}\, a_{l\,j}\, f(i,\, q)\, f^*(j,\, q)$$

$$= \frac{\pi\, Z^2\, \alpha^3}{4\alpha_0^2\, n\, |\omega|^8} \sum_{i,\,j} a_{l\,i}\, a_{l\,j}\, \frac{\omega^{*\,4|i-j|}}{|\omega|^{4|i-j|}}$$

$$= \frac{\pi\, Z^2\, \alpha^3}{4n a_0^2\, |\omega|^8} \sum_{i,\,j} a_{l\,i}\, a_{l\,j}\, \frac{R_e\left[\omega^{*\,4|i-j|}\right]}{|\omega|^{4|i-j|}}, \qquad (49)$$

where R_e stands for the real part of $\omega^{*\,4|i-j|}$.

When a binomial expansion is made of this quantity in terms of α and q, (Cf. Eq. (10)), we obtain

$$|F(l,\, q)|^2 = \frac{64\, \pi\, Z^2\, \alpha^3}{n a_0^2 (\alpha^2 + q^2)^4} \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} \sum_{\lambda=0}^{2|i-j|} (-)^\lambda a_{l\,i}\, a_{l\,j} \binom{4|i-j|}{2\lambda} \frac{\alpha^{4|i-j|-2\lambda}\, q^{2\lambda}}{(\alpha^2 + q^2)^{2|i-j|}} \cdot$$

$$(50)$$

In similar way, through Eq. (30),

$$|G(l,\, q)|^2 = \frac{16\, \pi\, Z^2\, \alpha^3}{n(\alpha^2 + q^2)^2} \sum_{i,\,j,\,\lambda} (-)^\lambda a_{l\,i}\, a_{l\,j} \binom{4|i-j|}{2\lambda} \frac{\alpha^{4|i-j|-2\lambda}\, q^{2\lambda}}{(\alpha^2 + q^2)^{2|i-j|}} \qquad (51)$$

By making use of Eqs. (27, 28) and making the expansion

$$q^{2\lambda} = (\rho^2 + \beta^2)^\lambda = \sum_{\mu=0}^{\lambda} \binom{\lambda}{\mu} \beta^{2(\lambda-\mu)}\, \rho^{2\mu} \qquad (52)$$

in Eqs. (50, 51), keeping in mind Eq. (32), we obtain the capture cross section with the initial states $n\,l$ and the final states $n'\,l'$, averaged over the initial states and summed over the final states. This is given by

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$$\sigma(nl, n'l') = \frac{1}{2\pi(2l+1)p^2} \int_0^\infty |F(l, q)|^2 \times |G(l', q')|^2 \, \rho \, d\rho$$

$$= \frac{2^9 \pi (ZZ')^2 (a a')^3}{(2l+1) a_0^2 p^2 n n'} \sum_\gamma \sum_{\gamma'} B(\gamma) B(\gamma') \int_0^\infty \frac{\rho^{2(\mu+\mu')+1} \, d\rho}{(\alpha^2 + \beta^2 + \rho^2)^{2(3+|i-j|+|i'-j'|)}} ,$$

where   (53)

$$B(\lambda) = (-)^\lambda \, a_{l_i} \, a_{l_j} \begin{pmatrix} 4|i-j| \\ 2\lambda \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \alpha^{4|i-j|-2\lambda} \beta^{2(\lambda-\mu)} , \qquad (54)$$

γ stands for the set of 4 integers i, j, λ, μ which take on the following values:

$$\left. \begin{aligned} i &= 0, 1, 2, \ldots, n-1 \quad ; \\ j &= 0, 1, 2, \ldots, n-1 \quad ; \\ \lambda &= 0, 1, 2, \ldots, 2|i-j| \; ; \\ \mu &= 0, 1, 2, \ldots, \lambda. \end{aligned} \right\} \qquad (55)$$

The integral appearing in Eq. (53) is of the form

$$I(M, N) = \int_0^\infty \frac{\rho^{2M+1} \, d\rho}{(b^2 + \rho^2)^N} , \qquad (56)$$

which after integration by parts yields

$$I(M, N) = \begin{pmatrix} N-1 \\ M \end{pmatrix}^{-1} I(0, N-M)$$

$$= \frac{1}{2} (M+1)^{-1} \begin{pmatrix} N-1 \\ M+1 \end{pmatrix}^{-1} b^{-2(N-M-1)} . \qquad (57)$$

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In this way we obtain

$$\sigma(n\ell, n'\ell') = \pi a_0^2 \, \frac{2^8 \, (ZZ')^5}{(2\ell + 1) \, (nn')^4 \, p^2} \cdot \frac{1}{[(\alpha^2 + \beta^2) \, a_0^2]^5}$$

$$\times \sum_{\gamma} \sum_{\gamma'} \frac{B(\gamma) \, B(\gamma')}{(1 + \mu + \mu') \binom{5 + 2(|i - j| + |i' - j'|)}{1 + \mu + \mu'} (\alpha^2 + \beta^2)^{2(|i - j| + |i' - j'|) - (\mu + \mu')}}$$

(58)

By introducing the dimensionless quantity

$$C(\gamma) = (\alpha^2 + \beta^2)^{-2|i - j| + \mu} \, B(\gamma)$$

$$= (-)^\gamma \, a_{\ell_i} \, a_{\ell_j} \binom{4|i - j|}{2\lambda} \binom{\lambda}{\mu} \frac{\alpha^{4|i - j| - 2\lambda} \, \beta^{2(\lambda - \mu)}}{(\alpha^2 + \beta^2)^{2|i - j| - \mu}} \,,$$

(59)

we finally get

$$\sigma(n\ell, n'\ell') = \pi a_0^2 \, \frac{2^8 \, (ZZ')^5}{(2\ell + 1) \, (nn')^4 \, p^2} \cdot \frac{1}{[(\alpha^2 + \beta^2) \, a_0^2]^5}$$

(60)

$$\times \sum_{\gamma} \sum_{\gamma'} (1 + \mu + \mu')^{-1} \binom{5 + 2(|i - j| + |i' - j'|)}{1 + \mu + \mu'}^{-1} C(\gamma) C(\gamma')$$

with γ defined by Eq. (55), and α and β given by Eqs. (1) and (16).

Since $\sigma(n\ell, n'\ell')$ does not change by the interchanges of i and j, and i' and j', Eq. (60) can be written alternatively as

$$\sigma(n\ell, n'\ell') = \pi a_0^2 \, \frac{2^8 \, (ZZ')^5}{(2\ell + 1) \, (nn')^4 \, p^2} \cdot \frac{1}{[(\alpha^2 + \beta^2) \, a_0^2]^5}$$

$$\times \sum_{\gamma} \sum_{\gamma'} [2 - \delta(i, j)] \, [2 - \delta(i', j')] \, (1 + \mu + \mu')^{-1} \binom{5 + 2(i - j + i' - j')}{1 + \mu + \mu'} C(\gamma) \, C(\gamma') \,,$$

(60')

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where $\delta(i, j)$ is the Kronecker delta, and summation over the indices is the same as given by Eq. (55) except that now

$$\left.\begin{array}{l} j = 0,\ 1,\ 2,\ \cdots,\ i; \\ \\ j' = 0,\ 1,\ 2,\ \cdots,\ i'. \end{array}\right\} \tag{55'}$$

If N be the number of the terms in the summations expressed by γ in Eq. (60'), it is easy to show that

$$N = \frac{1}{6} n^2 (n + 1) (n + 2). \tag{61}$$

Then the total number of terms in Eq. (60') is NN'.

When the initial state is the ground state, Eq. (60') reduces to, omitting the primes for convenience,

$$\sigma(1s, n\ell) = \pi a_0^2 \frac{2^8 (ZZ')^5}{n^4 p^2} \cdot \frac{1}{[(\alpha^2 + \beta^2) a_0^2]^5}$$

$$\times \sum_{i=0}^{n-1} \sum_{j=0}^{i} \sum_{\lambda=0}^{2(i-j)} \sum_{\mu=0}^{\lambda} [2 - \delta(i, j)] \frac{(-)^\lambda \dbinom{4(i-j)}{2\lambda}\dbinom{\lambda}{\mu}}{(1 + \mu)\dbinom{5 + 2(i-j)}{1 + \mu}} \cdot \frac{\alpha^{4(i-j)-2\lambda} \beta^{2(\lambda-\mu)}}{(\alpha^2 + \beta^2)^{2(i-j)+\mu}}. \tag{62}$$

The following simple formulas are obtained for the electron capture cross sections with the ground state as the initial state and the sublevels of $n = 1, 2, 3$ as the final states. Introducing

$$A = \frac{\alpha^2}{\alpha^2 + \beta^2}, \tag{63}$$

with α and β referring to the final states (Cf. Eqs. (1, 28), and

$$\sigma_0 = 2^8 (Z/Z')^5 p^{-2} A^5 (\pi a_0^2), \tag{64}$$

we obtain

(i)
$$\sigma(1s, 1s) = \frac{1}{5} \sigma_0,$$
(65)

in agreement with the value given by Bates and Dalgarno[8].

(ii)
$$\sigma(1s, 2s) = 2\sigma_0 \left(\frac{2}{5} - \frac{4}{3} A + \frac{8}{7} A^2 \right),$$
(66)

$$\sigma(1s, 2p) = 2\sigma_0 \left(\frac{4}{3} A - \frac{8}{7} A^2 \right),$$
(67)

$$\sigma(1, 2) = \sigma(1s, 2s) + \sigma(1s, 2p) = \frac{4}{5} \sigma_0.$$
(68)

(iii)
$$\sigma(1s, 3s) = 3\sigma_0 \left(\frac{3}{5} - \frac{16}{3} A + \frac{352}{21} A^2 - \frac{64}{3} A^3 + \frac{256}{27} A^4 \right),$$
(69)

$$\sigma(1s, 3p) = 3\sigma_0 \left(\frac{16}{3} A - \frac{160}{7} A^2 + 32 A^3 - \frac{128}{9} A^4 \right),$$
(70)

$$\sigma(1s, 3d) = 3\sigma_0 \left(\frac{128}{21} A^2 - \frac{32}{3} A^3 + \frac{128}{27} A^4 \right),$$
(71)

$$\sigma(1, 3) = \sigma(1s, 3s) + \sigma(1s, 3p) + \sigma(1s, 3d) = \frac{9}{5} \sigma_0.$$
(72)

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APPENDIX I

Classical Momentum Distribution of a Bound Particle
in a Coulomb Field

Assume a bound particle of charge $-e$, mass m and momentum $\mathbf{p}$ in the field of a nucleus of charge Ze. The conservation of energy requirement is that

$$E = \frac{p^2}{2m} - \frac{Ze^2}{r} , \tag{A1}$$

with E the energy of the particle and r its distance from the origin. We recognize that the density of the particle in phase space is given by

$$N\delta\left(E - \frac{p^2}{2m} + \frac{Ze^2}{r}\right),$$

with N the normalization constant determined by the equation

$$N \int \delta\left(E - \frac{p^2}{2m} + \frac{Ze^2}{r}\right) \, d\mathbf{r} \, d\mathbf{p} = 1. \tag{A2}$$

On the other hand if the momentum density between $\mathbf{p}$ and $\mathbf{p} + d\mathbf{p}$ is given by $D(\mathbf{p})$, we must have

$$\int D(\mathbf{p}) \, d\mathbf{p} = 1 . \tag{A3}$$

Combining Eqs. (A2) and (A3) we obtain

$$D(\mathbf{p}) = N \int \delta\left(E - \frac{p^2}{2m} + \frac{Ze^2}{r}\right) \, d\mathbf{r}$$

$$= \frac{\int \delta\left(E - \frac{p^2}{2m} + \frac{Ze^2}{r}\right) \, d\mathbf{r}}{\int \delta\left(E - \frac{p^2}{2m} + \frac{Ze^2}{r}\right) \, d\mathbf{r} \, d\mathbf{p}} . \tag{A4}$$

Below we evaluate the integrals occurring in (A4). Introducing

$$x = E - \frac{p^2}{2m} + \frac{Ze^2}{r} \, , \tag{A5}$$

we obtain

$$\int \delta \left(E - \frac{p^2}{2m} + \frac{Ze^2}{r} \right) d\mathbf{r} = 4\pi \int_{E-p^2/2m}^{\infty} \frac{(Ze^2)^3 \, \delta(x)}{\left[x - E + \frac{p^2}{2m} \right]^4} \, dx$$

$$= \frac{4\pi \, (Ze^2)^3}{\left[\frac{p^2}{2m} - E \right]^4} \, . \tag{A6}$$

Consequently

$$\int \delta \left(E - \frac{p^2}{2m} + \frac{Ze^2}{r} \right) d\mathbf{r} \, d\mathbf{p} = 16 \, \pi^2 \, (Ze^2)^3 \int_0^{\infty} \frac{p^2 \, dp}{\left[\frac{p^2}{2m} - E \right]^4}$$

$$= 16 \, \pi^2 \, (Ze^2)^3 \cdot \frac{\pi (2m)^{3/2}}{32 \, (-E)^{5/2}} \, . \tag{A7}$$

In this way we obtain

$$D(\mathbf{p}) = \frac{8 \, (-2m \, E)^{5/2}}{\pi^2 \, (p^2 - 2m \, E)^4} \, , \tag{A8}$$

which is the desired relationship. It is seen that $D(\mathbf{p})$ is a scalar and independent of the direction of $\mathbf{p}$.

To show the agreement of this equation with the quantum mechanical momentum distribution, following the text we introduce the propagation vector $\mathbf{q}$ related to $\mathbf{p}$ by

$$\mathbf{p} = \hbar \, \mathbf{q} \, . \tag{A9}$$

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We then obtain

$$D(\mathbf{q}) \, d\mathbf{q} = D(\mathbf{p}) \, d\mathbf{p} = \hbar^3 \, D(\mathbf{p}) \, d\mathbf{q}. \qquad \text{(A10)}$$

According to Bohr-Sommerfeld classical quantization formula:

$$E = -\frac{Z^2 \, e^2}{n^2 \, a_0} = -\frac{\hbar^2 \, \alpha^2}{2m} \, ,$$

α defined by Eq. (1). In this way we obtain from (A8), (A9), (A10),

$$D(\mathbf{q}) = \frac{8 \, \hbar^3 \, (\hbar\alpha)^5}{\pi^2 \hbar^8 \, (\alpha^2 + q^2)^4} = \frac{8 \, Z^2 \, \alpha^3}{n^2 \, \pi^2 \, a_0^2 \, (\alpha^2 + q^2)^4} \, , \qquad \text{(A11)}$$

in agreement with Eq. (1).

APPENDIX II

The Elements of the Transformation Matrix
between the Spherical and the Parabolic Wave Functions

We require the transformation matrix which for a given principal quantum number n transforms the n states with m = 0 in the spherical coordinates to another set of n states in the parabolic coordinates. The simplest way to find the transformation matrix is by noticing that the matrix elements of interaction of an electric field with the hydrogen atom, taken with the unperturbed wave function of the atom, are diagonal in the parabolic coordinates representation. Let ϵ be this matrix and let A be the transformation matrix. We must then have

$$A \, H' \, A^{-1} = \epsilon, \tag{A12}$$

where H' is the interaction matrix in spherical coordinates. ϵ is given by[18]

$$\epsilon_{ij} = - \delta(i, j) \frac{3}{2} n e \, F \, a_0 \, (2j + 1 - n),$$

$$j = 0, \ 1, \ 2, \ \cdots, \ n, \tag{A13}$$

with F the strength of the electric field. Similarly through Eq. (38) we can write

$$H'_{ij} = - eF \int \varphi^*_{ni0} (\mathbf{r}) \, r \cos \theta \, \varphi_{nj0}(\mathbf{r}) \, d\mathbf{r}$$

$$= - eF \int_0^\infty R_{ni}(r) \, R_{nj}(r) \, r^3 \, dr \times \int Y_{i0}(\Omega) \, Y_{j0}(\Omega) \cos \theta \, d\Omega. \tag{A14}$$

Now[19]

$$\int Y_{i0}(\Omega) Y_{j0}(\Omega) \cos\theta \, d\Omega = 2\pi \left(\frac{2i+1}{4\pi}\right)^{1/2} \left(\frac{2j+1}{4\pi}\right)^{1/2} \int_{-1}^{+1} P_i^0(\mu) P_j^0(\mu) \mu \, d\mu$$

$$= \frac{1}{2} \left(\frac{2j+1}{2i+1}\right)^{1/2} \int_{-1}^{+1} [i \, P_{i-1}^0 \, P_j^0 + (i+1) \, P_{i+1}^0 \, P_j^0] \, d\mu$$

$$= \frac{i \, \delta(i, j+1)}{[(2i+1)(2i-1)]^{1/2}} + \frac{(i+1) \, \delta(i+1, j)}{[(2i+1)(2i+3)]^{1/2}} . \tag{A15}$$

Also[20]

$$\int_0^\infty R_{ni}^{(r)} R_{ni-1}^{(r)} \, r^3 \, dr = \frac{3}{2} \, a_0 \, n \, \sqrt{n^2 - i^2} . \tag{A16}$$

In this way we obtain

$$H'_{ij} = -\frac{3}{2} \, ne \, F \, a_0 \, [C_i \, \delta(i, j+1) + C_{i+1} \, \delta(i+1, j)], \tag{A17}$$

with

$$C_i = \frac{i \, \sqrt{n^2 - i^2}}{[(2i+1)(2i-1)]^{1/2}} . \tag{A18}$$

Eq. (A12) can now be written

$$\sum_l A_{il} \, H'_{lj} = \epsilon_{ii} \, A_{ij} , \tag{A19}$$

which by means of Eqs. (A13), (A17) reduces to

$$A_{i\,j+1} \, C_{j+1} + A_{i\,j-1} \, C_j = (2i + 1 - n) \, A_{ij} . \tag{A20}$$

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This is a recursion relationship for **A** by means of which all the elements of a row of **A** can be found once the first element of the row is given.

The unitary condition on **A** gives

$$\sum_{j=0}^{n-1} A_{ij}^2 = 1,$$ (A21)

where we have assumed that the elements of **A** are real and if a solution for **A** is found our assumption is justified.

Eqs. (A20) and (A21) are sufficient for the determination of **A** for any given n. This has been done for n = 1, 2, 3, 4, 5. In the text the inverse of **A** is needed. Let **a** be the inverse of **A**,

$$\mathbf{a} = \mathbf{A}^{-1} = \tilde{\mathbf{A}},$$ (A22)

with $\tilde{\mathbf{A}}$ the transpose of **A**. The elements of **a** for n = 1, 2, 3, 4, 5 are given below.

$$\mathbf{a}(1) = 1, \qquad \mathbf{a}(2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix},$$

$$\mathbf{a}(3) = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ -\sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{3}{2}} \\ \sqrt{\frac{1}{2}} & -\sqrt{2} & \sqrt{\frac{1}{2}} \end{pmatrix},$$

$$\mathbf{a}(4) = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ \frac{-3}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & \frac{3}{\sqrt{5}} \\ 1 & -1 & -1 & 1 \\ \frac{-1}{\sqrt{5}} & \frac{3}{\sqrt{5}} & \frac{-3}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{pmatrix},$$

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$$\mathbf{a}(5) = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -\sqrt{2} & -\sqrt{\frac{1}{2}} & 0 & \sqrt{\frac{1}{2}} & \sqrt{2} \\ \sqrt{\frac{10}{7}} & -\sqrt{\frac{5}{14}} & -\sqrt{\frac{10}{7}} & -\sqrt{\frac{5}{14}} & \sqrt{\frac{10}{7}} \\ -\sqrt{\frac{1}{2}} & \sqrt{2} & 0 & -\sqrt{2} & \sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{14}} & -\sqrt{\frac{8}{7}} & \sqrt{\frac{8}{7}} & -\sqrt{\frac{8}{7}} & \sqrt{\frac{1}{14}} \end{pmatrix}$$

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